Developing Extinction Criteria for Fires

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Overview

Introduction

- Poorly Ventilated Fires
- Extinction Problem Formulation

Kinematic Scale Analysis for Fire

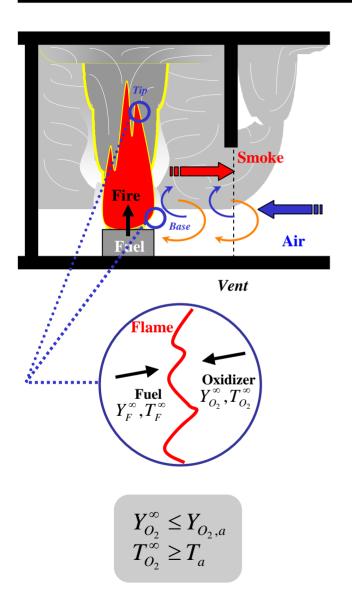
Extinction Analysis for Fire

- Experiments
- OPPDIF Simulations
- Asymptotic Theory
- Critical Damköhler Number
- Critical Scalar Dissipation Rate Model

Summary and Future Work



Introduction: Poorly Ventilated Fires



Extinction Effects

- Extinction places raw fuel in smoke increasing its toxicity and contributing to CO production.
- Local or global vitiation (typical of compartment fires) makes flame vulnerable to extinction.

Extinction Criteria

- In fire, this vulnerability typically expressed in terms of a global O₂ concentration.
- Recognizing that extinction is a local flame phenomenon (Simmons and Wolfhard, 1957) and later (Ishizuka and Tsuji, 1981) established a criterion where extinction occurs when $Y_{o_2}^{\infty} < 0.16$ at 300K for weakly strained methane flames.

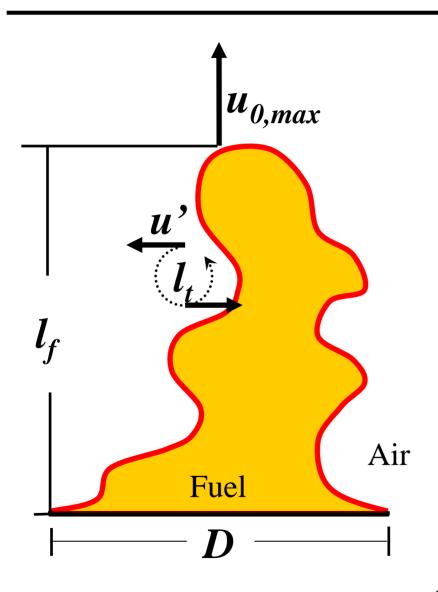


Introduction: Extinction Problem Formulation

- Strictly, extinction criteria must include composition, temperature, and flow effects.
- It is necessary to assess the relative importance of these effects and apply them to fire simulation tools.

Extinction Analysis Local Flame Flamelet $Y_{O_2}^{\infty}, T_{O_2}^{\infty}, Z^+ = 0$ Oxidizer **Fuel** $Y_f^{\infty}, T_f^{\infty}, Z^+ = 1$ Determine convenient extinction criteria at these flow conditions.

Kinematic Scales in Fires



- Use well known and experimentally validated scaling laws to predict large scale motions.
- Use Kolmogorov scaling arguments to predict small scale motions (local strain rate) from the large scale motions.
- Analytic solutions from asymptotic analysis predict a characteristic scalar dissipation rate.



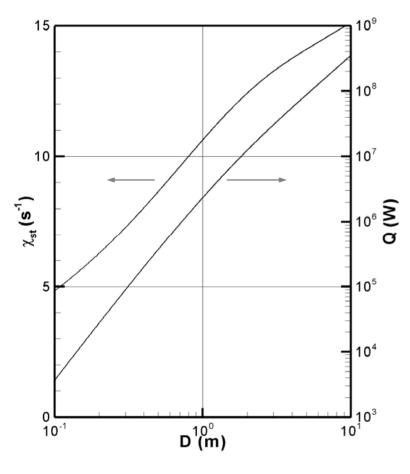
Kinematic Scales in Fires

Fire Scale	Integral Scale	Kolmogorov Scale
D	$l_{t} = 0.5D$	$\eta_k = l_t \operatorname{Re}_t^{-3/4}$
$\dot{Q} = \Delta h_c \frac{\pi D^2}{4} \dot{m}_{\infty}'' (1 - e^{-kBD})$	$u' = 0.3u_{0,\text{max}}$	$V_k = u' \operatorname{Re}_t^{-1/4}$
$u_{0,\text{max}} = 0.54 \left(\Delta T_0 \frac{\dot{Q}}{1000}\right)^{1/5}$	$Re_{t} = \frac{u'l_{t}}{v}$	$a_t = \frac{V_k}{\eta_k}$

$$\chi_{st} = \varphi(a_t/\pi) \exp\left\{-2\left[\operatorname{erfc}^{-1}(2Z_{st})\right]^2\right\}$$



Kinematic Scales in Fires

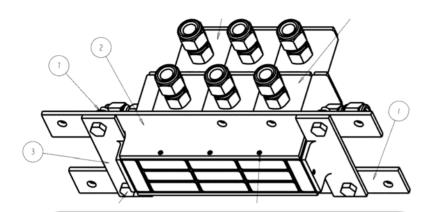


Heptane Pool Fire

- Characteristic mean scalar dissipation rate at the flame tip as a function of pan Diameter (and Fuel specific parameters).
- Velocity predictions compare well with 1m diameter Methane flame measurements by (Tieszen, 2002).
- Another region of interest is the base of the flame where
 - Large scale laminar mixing dominates
 - We are examining the effect with direct numerical simulation



Experimental Approach



Burner Features

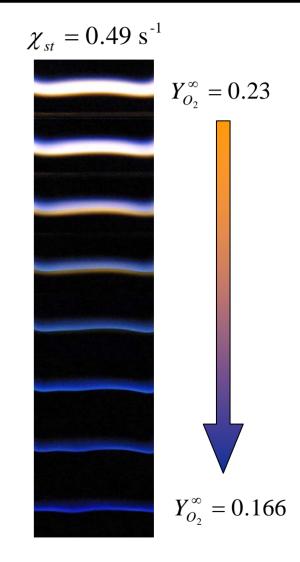
- Low strain flames: $(12 s^{-1} 75 s^{-1})$
- Vitiated and heated reactant inlet.

$$-$$
 300 K < $T_{O2,\infty}$ < 600 K

$$-0.0 < Y_{O2,\infty} < 0.23$$

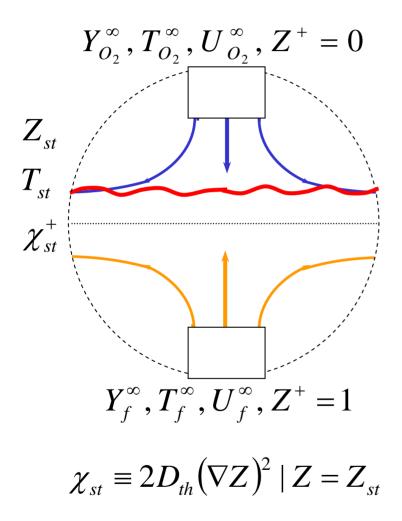
$$-0.0 < Y_{f,\infty} < 1.0$$

Nitrogen co-flow flame isolation





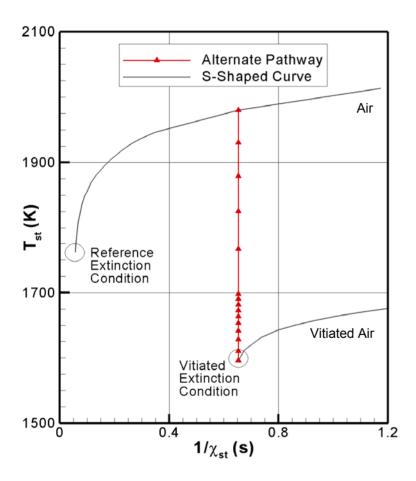
OPPDIF Simulation Approach



- CHEMKIN 4.1 OPPDIF Solver
 - Steady state
 - GRI 3.0 Chemical Kinetics
 - Adiabatic (no radiation)
- Uses the von Karman similarity transformation to simplify the 3-D flame to 1-D equations.
- High resolution allows for exact determination of key parameters such as scalar dissipation rate and temperature at $Z = Z_{st}$.



Extinction Criteria for Fires



Pathways to Extinction

Classical S-Shaped Curve

- Constant reactant properties
- Extinction by increasing strain

Alternative pathway

- Constant scalar dissipation rate
- Extinction by dilution of reactants
- Variable temperature reactants are also examined

Comparing extinction conditions

- Flame temperature
- Scalar dissipation rate



Critical Scalar Dissipation Rate Models

Asym	ptotic	Theory	

Da Argument in Study

(Williams, 1975); (Peters, 1983); (Puri and Seshadri, 1986)

$$Da_{crit} = \frac{t_{mix}}{t_{chem}} \approx \frac{\chi_{st}^{-1}}{A \exp\left(\frac{T_a}{T_{st}}\right)}$$

Conventional

$$\chi_{st} = \left(a_g / \pi\right) \exp \left\{-2\left[\operatorname{erfc}^{-1}(2Z_{st})\right]^2\right\}$$

$$\chi_{st} = \varphi (Z_f - Z_{O_2})^2$$

$$(a_g / \pi) \exp \left\{ -2 \left[\operatorname{erfc}^{-1} (2Z_{st}) \right]^2 \right\}$$

$$\ln\left(\frac{f(Z_{st})\chi_{st}}{T_{st,BS}^{5}}\right) = -\frac{T_{a}}{T_{st,BS}} + \ln K$$

$$\ln \chi_{st} = -\frac{T_a}{T_{st,BS}} + \ln \left(Da_{crit}^{-1} A^{-1} \right)$$

$$T_{st,BS} = T_{O_2}^{\infty} Z_{st} + T_f^{\infty} (1 - Z_{st}) + \frac{\Delta h_c}{C_p} Y_f^{\infty} Z_{st}$$



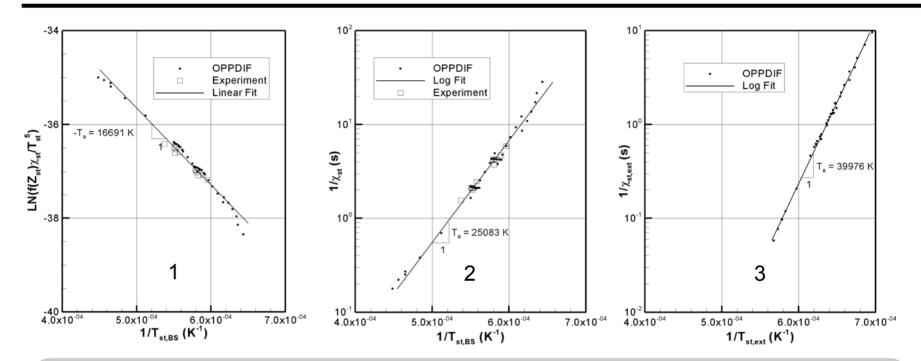
Critical Scalar Dissipation Rate Models

Asymptotic Theory	Da Argument in Study
Model 1	Model 2
$\frac{\chi_{st}}{\chi_{st}^{ref}} = \frac{f(Z_{st}^{ref})}{f(Z_{st})} \left(\frac{T_{st,BS}}{T_{st,BS}^{ref}}\right)^{5}$ $\exp\left[-T_{a}\left(\frac{1}{T_{st,BS}} - \frac{1}{T_{st,BS}^{ref}}\right)\right]$	$\frac{\chi_{st}}{\chi_{st}^{ref}} = \exp\left[-T_a \left(\frac{1}{T_{st,BS}} - \frac{1}{T_{st,BS}^{ref}}\right)\right]$
$\chi_{st}^{ref} = 6.96 \mathrm{s}^{-1}$	$\chi_{st}^{ref} = 11.23 \mathrm{s}^{-1}$

Normalization by a reference condition gives the model a convenient form



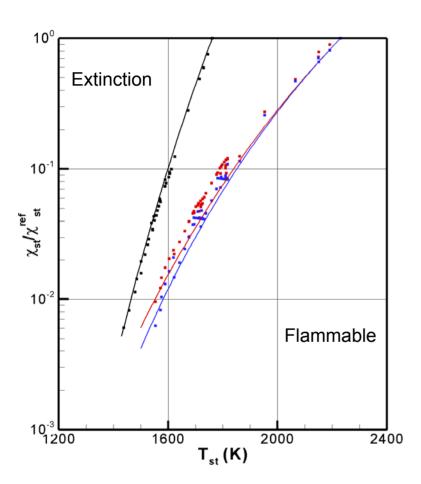
Determining Activation Temperatures



- **Model 1** Asymptotic analysis following the method of Puri and Seshadri using Burke-Schumann temperatures and the original equation for scalar dissipation rate.
- **Model 2** Critical Damköhler model using Burke-Schumann temperatures, and scalar dissipation rate from asymptotic analysis including density correction and renormalization.
- **Model 3** Numerical observation of extinction behavior follows the critical Damköhler number behavior.



Critical Scalar Dissipation Rate Models



Extinction Models

Model 1 (Red):

- Data from Conventional χ_{st}
- Asymptotic analysis approach

Model 2 (Blue):

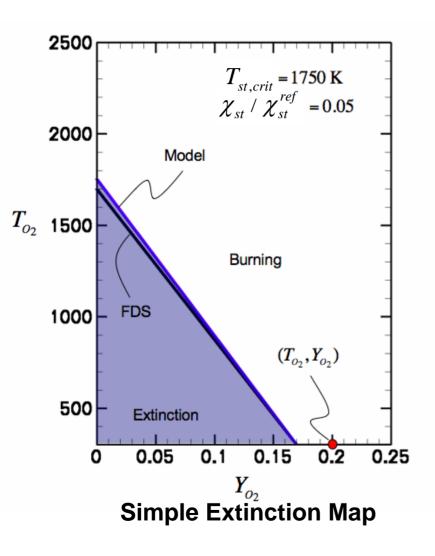
- Data from Corrected χ_{st}
- Critical Damköhler number approach
- Better agreement with χ_{st} and χ_{st} / χ_{st}^{ref} from Model 3 due to added correction factors

Model 3 (Black):

- Data from definition of χ_{st}
- Critical Damköhler number approach



Extinction Map



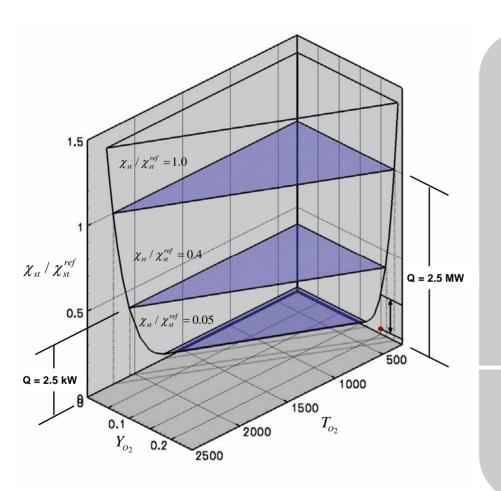
- Extinction map created by specifying $T_{st\ crit}$ or χ_{st} / χ_{st}^{ref} .
- FDS extinction map similar to current model at a low scalar dissipation rate (Model 2).
- Sample condition is vitiated, but still sufficient for burning.

Extinction Condition

$$Y_{O_2} < Y_{O_2,crit}$$



3D Extinction Map



- Extinction region grows with increasing scalar dissipation rate.
- Fire size determines range of possible scalar dissipation rates.
- This view provides detailed physical insight, but adds complexity to extinction model

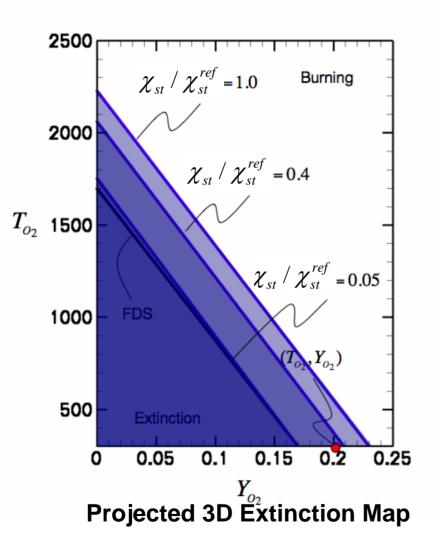
Extinction Condition

$$\chi_{st}/\chi_{st}^{ref} > (\chi_{st}/\chi_{st}^{ref})_{crit}$$

3D Extinction Map



Extinction Boundary Analysis



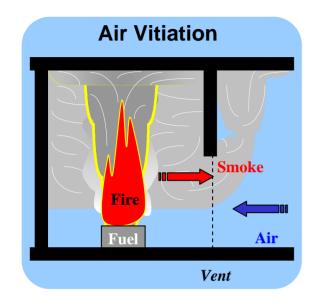
- 2D maps clearly reveal the effect of increased scalar dissipation rate.
- FDS map corresponds to a low and constant (one boundary) scalar dissipation rate assumption.
- Increasing fire size can expand the possible extinction conditions (flow dependent boundaries).
- The importance of radiation losses and fuel vitiation will be explored to determine if flow effects can be neglected.

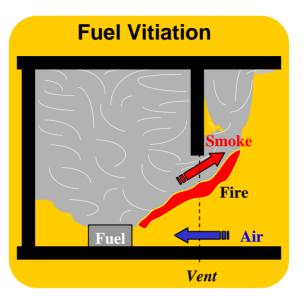


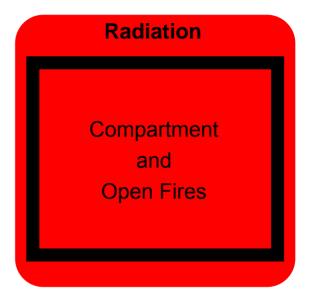
Summary of Current Work

- Developed an approach to characterize vitiated extinction in fires.
- Scaling argument indicates potentially significant scalar dissipation rates in large fires. (1m)
- Examined the application of three scalar dissipation rate extinction models considering Oxidizer vitiation.
- These models capture the essential physics of extinction but add unwanted complexity.
- The importance of radiation losses and fuel vitiation will be explored to determine if flow effects can be neglected.

Future Work







Burke-Schumann Critical Temperature Extinction Model

$$(T_{st} - T_c) = T_{o_2}^{\infty} Z_{st} + T_f^{\infty} (1 - Z_{st}) + Y_f^{\infty} \left(\frac{Z_{st}}{Z_{st}^0} \right) (1 - X_r) (T_{st}^0 - T_u) - T_c$$

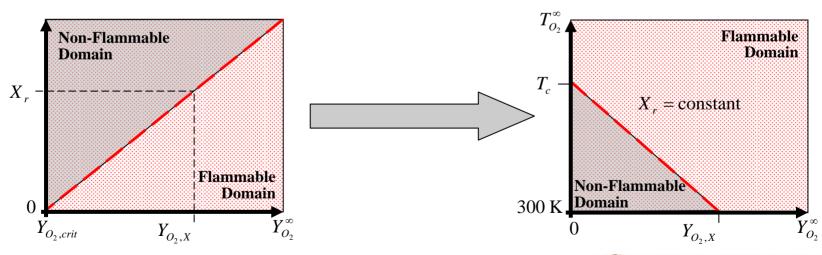
Extinction at
$$(T_{st} - T_c) \le 0$$



Future Work

Development

- Modify the extinction model to include fuel vitiation and radiation effects.
- Perform opposed flow experiments with imposed radiation losses and fuel vitiation to support model development.
- 2-D extinction maps can be derived from these variables in order to represent them in a similar way to the air vitiation case.
- Example for Radiation effects below:



Future Work

Validation

- Simulate Pool Fires (Hamins, 1993-1996) and Reduced-Scale Enclosure (RSE) Experiments performed by NIST.
- Evaluate the critical temperature model's ability to reproduce combustion efficiency to determine if neglecting flow effects is appropriate.

Thank You

